

Mathematical Modelling and Simulation of Multicomponent Distillation Column for Acetone-Chloroform-Methanol System

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Abstract

A steady state mathematical model was developed to describe the operation type of multicomponent distillation process using a plate-to-plate method involving Murphree plate efficiency. The developed model equations were applied to a ternary system of acetone-chloroform-methanol in a ten-stage distillation column. An algorithm for solving the operation type of this ternary distillation problem was presented. Numerical solutions were obtained via MATLAB using condenser's boundary condition as initial guess. The simulated results of the variations of temperature, activity coefficient and mole fractions of acetone, chloroform and methanol in the liquid, with number of theoretical stages in the 10-stage distillation column, conformed to the trends in the literature. The convergence behaviour of the method employed in this work showed that convergence was achieved within 7-10 iterations.

Keywords

Distillation; Plate-to-plate Method; Murphree Plate Efficiency; Ternary; Activity Coefficient; Convergence

Introduction

Distillation is by far the most widely practiced technique to separate mixtures of chemical species in petroleum, natural gas, liquid and chemical industries. It is a separation process that takes advantage of differences in boiling points in a number of vaporisation and condensation steps (Solomon, 1981). Brooks (1993) defined distillation column as a device used to separate components of a mixture using the thermodynamic properties of the components. A schematic diagram of a typical distillation unit with a single feed and two product streams is shown in Figure 1. The column itself is adiabatic. The initial mixture to be processed, known as the feed, is introduced somewhere near the middle of the column to a tray known as the feed tray, f . The feed tray

divides the column into a top (absorption/enriching/rectification) section and a bottom (stripping/exhausting) section. Heat is added to the bottom of the column as reboiler heat, Q_R , and removed at the top as the heat load of the condenser, Q_C . Essentially, components with lower boiling points will tend toward the top of the column as vapour and the components with higher boiling points will gravitate toward the bottom as liquid.

Hence, distillate, D , and bottoms, W , are removed from the top and bottom of the column respectively. Inside the tower, liquids and vapours are always at their bubble and dew points respectively so that the highest temperatures are at the bottom, the lowest at the top. The reboiler can be considered as a theoretical stage or tray. Thus, there are internal flows of vapour and liquid within the column as well as external flows of feeds and product streams, into and out of the column. The contact between vapour and liquid on a tray engenders heat and mass exchanges conducive to the separation goal of a distillation column. The entropy and molar flow between the liquid and vapour phases are complex phenomena. Convection, conduction and heat of vaporisation take place as the fluids flow through a stage, exchanging heat and mass.

Modelling and simulation of distillation columns are not new enterprises. The models used for distillation columns vary from the simple to the quite complex, depending on the nature of assumptions. The models described in the literature either contain algebraic loops or simplified assumptions that render the models ill-equipped for dynamic simulations (Brooks, 1993).

Multicomponent distillation calculations are classified as design or rating methods (Rao et al., 2005). In the former, the number of stages has to be determined given the recovery of key components whilst in the

latter, the composition of products has to be found given the number of stages in the enriching and stripping sections of the distillation column. Lewis et al. (1932) proposed a method of the stage-to-stage calculations for multicomponent distillation. To determine an approximate distillate composition, they considered that components lighter than light key will present in significant amounts only in the distillate and components heavier than heavy key in the bottom product. Assigning arbitrarily small amounts for the missing components, they proposed to compute the product compositions to initiate the stage-to-stage calculation and match the feed stage compositions computed from both sections. The discrepancy between the feed stages' compositions thus being computed was used to revise the products compositions. However, this method did not gain acceptance and currently there are no simple and robust design methods (Fidkowski et al., 1991). To avoid the arbitrary assignment of the missing components in the products, Thiele et al. (1933) proposed a method in which they preassigned the number of stages in each section of the column, and determined the product compositions. This method lends itself well to cast the component and enthalpy balances around the stages into elegant tridiagonal or block diagonal matrix equation(s).

Then, the Newton-Raphson method was used to find the compositions of products, and liquid and vapour streams in the column. The developments in this direction have led to the well-known Napthali-Sandholm method and its variants. To extend the domain of convergence and find multiple solutions, physical and mathematical homotopy-continuation methods were used. Ketchum (1979) integrated the relaxation method, proposed by Rose et al. (1958), into a variant of the Napthali-Sandholm method. These can be adopted for equilibrium and non-equilibrium stage models and reactive distillation. Hass (1992) reviewed the developments of these methods. These methods are robust and several commercial softwares have incorporated them for solving rating problems. The above methods are used for design as well, but the solutions of several runs of rating problems are required. Based on experience, using the Fenske-Underwood-Gilliland short-cut method, one obtains the near about solution for the design problem. This solution can be used to minimize the rating runs required to arrive at the solution of design problem. This, perhaps, constitutes the widely design method at present.

The design method had been previously revised in the

context of azeotropic distillation to determine rigorously the minimum reflux. Levy et al. (1985) and Julka et al. (1993) proposed methods for the direct and indirect splits of ternary and multicomponent mixtures based on the 'distillation' lines and showed that they could be used for any split of multicomponent systems. Brooks (1993) worked on modelling and simulation of a distillation column using bond graphs. The structure and the equations that represent a sieve-tray distillation column were explored using bond graphs. They concluded that creating a truly dynamic, rigorous bond graph model of a distillation column requires more fundamental research. Thong et al. (2000) (2001) proposed methods using the 'stage-composition' lines. In a way, these are similar to the Lewis-Matheson method, but the match is found either geometrically or by a 'tuning' algorithm.

Jimenez et al. (2002) provided a basis for the estimation of liquid-phase activity coefficient of any component i , from the molecular volume fractions, Φ_i . The liquid-phase activity coefficients can be individually differentiated in the combinatorial part, which includes the geometric significance for combining molecules of different shapes and sizes, and the residual part, which includes the energy parameters. Rao et al. (2005) worked on simple design method for multicomponent distillation columns.

A simple design method in which the stage-to-stage calculations were initiated from the feed stage with the feed compositions was presented. The method permits the use of component or matrix tray efficiencies or the non-equilibrium-stage model to estimate the number of stages. The convergence was achieved in all the cases within 3-20 iterations taking CPU time in the order of 100th of a second on a PC with a Pentium IV processor. Zuzana et al. (2007) examined the impact of mathematical model selection on prediction of steady state behaviour of a reactive distillation column. The objective of their paper was to compare the equilibrium (EQ) and non-equilibrium (NEQ) models of a reactive distillation column, focusing on the phenomenon of multiple steady states. It was concluded in their work that the EQ and NEQ models showed qualitative different responses to feed flow rates disturbances of methanol and butanes, predicted different start-up strategy to achieve higher steady states. Minh et al. (2009) introduced a calculation procedure for modelling and control simulation of a condensate distillation column based on the energy balance structure. The mathematical modelling simulation was accomplished over three

phases: the basic nonlinear model, the full-order linearized model and the reduced-order linear model.

Recently, Frau et al. (2010) investigated estimation model design for a multicomponent distillation column with temperature measurements. This approach was applied through simulations to an industrial-type six-component column. It was concluded that the estimation task could be performed with much less (57) ODEs compared to the standard three (2849 ODEs) and six (17390 ODEs) component Extended Kalman Filters. Truong et al. (2011) reviewed some techniques of modelling and simulation of distillation columns and described a model for a lab-scale binary continuous distillation column with the focus was on the dynamic behaviour of the product compositions under feed disturbances. The simulation results showed that the composition responses to disturbances were close to the response of a first order system. Popoola et al. (2013) did comprehensive review of expert system design of crude oil distillation column as an industrial application of distillation column using the neural networks model. It was observed that the use of dynamic mathematical models was challenging due to their time dependency; and then they proposed the use of back-propagation algorithm involving error minimal method to replace convergence problem experienced by previous researchers.

The objective of this study was to develop a steady state mathematical model for multicomponent distillation column using plate-to-plate method involving Murphree plate efficiency and a condition of plate matching at the vapour on the feed plate. Hence, an algorithm was proposed for solving the operation type of multicomponent distillation problem with a view to determining the liquid composition and temperature profile, variation of activity coefficient with number of stages, and the number of iterations required to achieve convergence.

Scope

Most of the calculation methods used in the studies of distillation process were developed by assuming a so-called ideal stage. In this study, a steady state mathematical model was developed for the operation type of multicomponent distillation process by use of a plate-to-plate method involving Murphree plate efficiency and a condition of plate matching at the vapour composition on the feed plate in contrast to the θ 's method proposed by Holland et al. (1983), where plate matching implies that the liquid composition on the feed plate obtained by calculation steps for both

enriching and stripping sections of the column must be equal for all components.

The Mathematical Model

The multicomponent distillation column was modelled using the plate-to-plate calculation technique involving Murphree plate efficiency and a condition of plate matching at the vapour composition on the feed plate. Figure 1 shows a typical distillation column, whereby the feed F , is introduced on plate f , and overhead and bottom products are withdrawn as distillate, D , and bottoms, W , respectively. The feed tray divides the column into a top (absorption/enriching/rectification) section and a bottom (stripping/exhausting) section. The plates are numbered from the top through the feed plate to the bottom of the column, as shown in Figure 1.

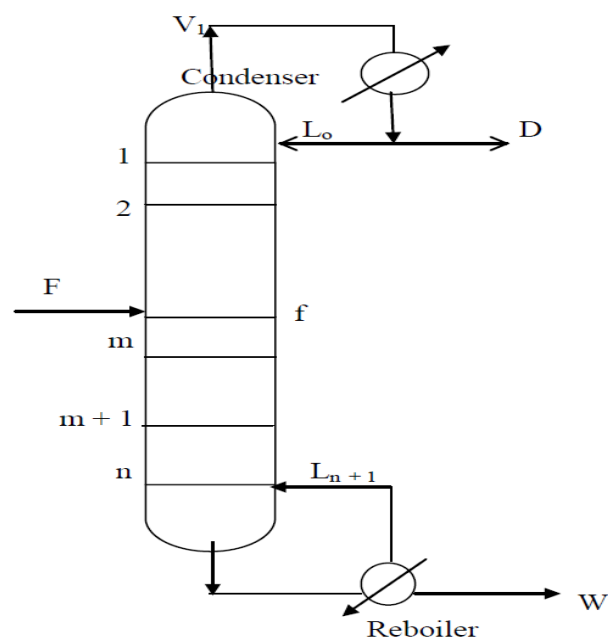


FIGURE 1 A TYPICAL DISTILLATION COLUMN.

The Murphree plate efficiency, $E_{j,n}^{MV}$, is defined by:

$$E_{j,n}^{MV} = \frac{y_{j,n} - y_{j,p}}{y_{j,n}^* - y_{j,p}}, j = 1, 2, \dots, M; n = 1, 2, \dots, N \quad (1)$$

where $p = n + 1$ for the enriching section and $p = N - f$ for the stripping section.

The operating line of the enriching section is given by:

$$y_{j,n+1} = \frac{R}{R+1} x_{j,n} + \frac{x_{j,D}}{R+1} \quad (2)$$

where R is the reflux ratio $\left(= \frac{L_0}{D} \right)$. Equimolar rates of flow of liquid and vapour are respectively assumed in the enriching section, that is: $L_1 = L_2 = \dots = L_n$ and $V_1 = V_2 = \dots = V_{n+1}$.

Using equations (1) and (2) to eliminate $y_{j,n+1}$, and

noting that the equilibrium relationship is given by:

$$y_{j,n}^* = K_{j,n} x_{j,n} \quad (3)$$

the following equation is obtained:

$$x_{j,n} = \frac{y_{j,n} - \alpha_2 x_{j,D} (1 - E_{j,n}^{MV})}{\alpha_1 (1 - E_{j,n}^{MV}) + E_{j,n}^{MV} K_{j,n}} \quad (4)$$

so that

$$\sum_{j=1}^M x_{j,n} = \sum_{j=1}^M \left[\frac{y_{j,n} - \alpha_2 x_{j,D} (1 - E_{j,n}^{MV})}{\alpha_1 (1 - E_{j,n}^{MV}) + E_{j,n}^{MV} K_{j,n}} \right] = 1.0 \quad (5)$$

where $\alpha_1 = \frac{R}{R+1}$ and $\alpha_2 = \frac{1}{R+1}$.

Generally, $K_{j,n}$ is given by a function of both activity coefficient (related to composition) and temperature thus:

$$K_{j,n} = \Phi(\gamma_{j,n}, T_n) \quad (6)$$

However, $K_{j,n}$ can be regarded as independent of composition for an ideal system. The values of $x_{j,D}$, α_1 and α_2 can be assigned; and $y_{j,1}$ is determined by the boundary condition at the condenser. If the system is ideal, $x_{j,n}$ is calculated for the given values of $E_{j,n}^{MV}$ from equation (4) with $K_{j,n}$, which is obtained by solving equation (5). Then, $y_{j,2}$ is calculated by equation (2), and the stage-to-stage calculation is continued toward the feed plate as $j=2, 3, \dots, f$. If the system is non-ideal, and $E_{j,n}^{MV}$ is given by a complicated function of $y_{j,n}^*$ and $y_{j,p}$ (Yamada et al., 1980), two additional convergence loops are considered in the calculations mentioned above, where the minor loop is to correct the activity coefficient, $\gamma_{j,n}$, and the major loop is to correct the $E_{j,n}^{MV}$, as highlighted below.

The vapour pressures of pure components for a non-ideal system are correlated with temperature by Antoine equation:

$$\log p^o = A - \frac{B}{T + C} \quad (7)$$

where A , B and C are constants, different for each component and T is the temperature in °C. Hence,

$$K_{j,n} = \frac{\gamma_{j,n} \log^{-1} \left(A - \frac{B}{T + C} \right)}{p^o} \quad (8)$$

The activity coefficient of a ternary system is calculated by Margule's equation (Wohl, 1946):

$$\ln \gamma_{1,n} = A_{2,1} x_2^2 (1 - 2x_1) + 2A_{1,2} x_1 x_2 (1 - x_1) + A_{3,1} x_3^2 (1 - 2x_1)$$

$$+ 2A_{1,3} x_1 x_3 (1 - x_1) - 2A_{3,2} x_2 x_3^2 - 2A_{2,3} x_2^2 x_3 + \left[\frac{1}{2} (A_{1,2} + A_{2,1} + A_{2,3} + A_{3,1} + A_{3,2}) - Q' \right] (x_2 x_3 - 2x_1 x_2 x_3) \quad (9)$$

$$\ln \gamma_{2,n} = A_{3,2} x_3^2 (1 - 2x_2) + 2A_{2,3} x_2 x_3 (1 - x_2) + A_{1,2} x_1^2 (1 - 2x_2) + 2A_{2,1} x_1 x_2 (1 - x_2) - 2A_{1,3} x_1^2 x_3 - 2A_{3,1} x_1 x_3^2 +$$

$$\left[\frac{1}{2} (A_{1,2} + A_{1,3} + A_{2,3} + A_{3,1} + A_{3,2}) - Q' \right] (x_1 x_3 - 2x_1 x_2 x_3)$$

$$\ln \gamma_{3,n} = A_{1,3} x_1^2 (1 - 2x_3) + 2A_{3,1} x_1 x_3 (1 - x_3) + A_{2,3} x_2^2 (1 - 2x_3) + 2A_{3,2} x_2 x_3 (1 - x_3) - 2A_{2,1} x_1 x_2^2 - 2A_{1,2} x_1^2 x_2 +$$

$$\left[\frac{1}{2} (A_{1,2} + A_{1,3} + A_{2,1} + A_{2,3} + A_{3,1}) - Q' \right] (x_1 x_2 - 2x_1 x_2 x_3)$$

Next, consider the stripping section of the distillation column. The operating line of the stripping section is given by:

$$x_{j,n+1} = \frac{R'}{R' - 1} y_{j,n} + \frac{x_{j,W}}{R' - 1} \quad (12)$$

where R' is the reflux ratio at the bottoms $\left(= \frac{L_{n+1}}{W} \right)$.

The reboiler used in the bottoms is to be an ideal stage, $E_{W,j}^{MV} = 1$. The plate-to-plate calculation in the stripping section is continued upward toward the feed plate without any complicated procedure, since the values of $x_{j,n}$ and $y_{j,n-1}$ to calculate $y_{j,n}$ have already been obtained by the previous step.

The component material balance across the column is given by:

$$Fz_{j,F} = Dx_{j,D} + Wx_{j,W} \quad (13)$$

Convergence Method for Operation Type

The so-called operation type is to calculate $x_{j,D}$ and $x_{j,W}$ for the given operating conditions such as $Fx_{j,F}$ and R , and number of plates in the enriching and stripping sections, n and s respectively. When ideal column was assumed, $E_{j,W}^{MV} = 1$ for all plates and components. Holland et al. (1983) proposed the θ 's method to correct the values of $x_{j,D}$ and $x_{j,W}$ assumed, by satisfying the condition of "plate matching" and the component overall material balance, where plate matching implies that the liquid composition on the feed plate, $x_{j,f}$, obtained by calculation steps for both enriching and stripping sections must be equal for all components. However, this condition cannot be applied to the plate-to-plate method involving Murphree plate efficiency. This is because the value of $y_{j,n+1}$ ($= y_{j,f}^*$, determined by

calculation step of the stripping section) cannot be obtained in the calculation step of the enriching section. Therefore, in the plate-to-plate method involving the Murphree plate efficiency, plate matching must be made for a condition in which the vapour composition leaving the feed plate, $y_{j,f}$, calculated from both sections of the column must be equal to each other. Thus, equations to obtain the corrected values of $x_{j,D}$ and $x_{j,W}$ are as follows:

$$x_{j,D(co)} = \frac{FX_{j,F}}{D + W \left(\frac{x_{j,W}}{x_{j,D}} \right) \text{cal } \theta_1} \quad (14)$$

$$x_{j,W(co)} = \frac{FX_{j,F}}{W + D \left(\frac{x_{j,D}}{x_{j,W}} \right) \text{cal } \theta_2} \quad (15)$$

where θ_1 and θ_2 are determined by:

and $\left[\frac{x_{j,D}}{x_{j,W}} \right]_{\text{cal}}$ is given by:

$$\left[\frac{x_{j,D}}{x_{j,W}} \right]_{\text{cal}} = \left[\frac{x_{j,D(as)}}{x_{j,W(as)}} \right] \left[\frac{y_{j,f(w)}}{y_{j,f(D)}} \right] \quad (18)$$

The flow chart of the proposed method is given in Figure 2.

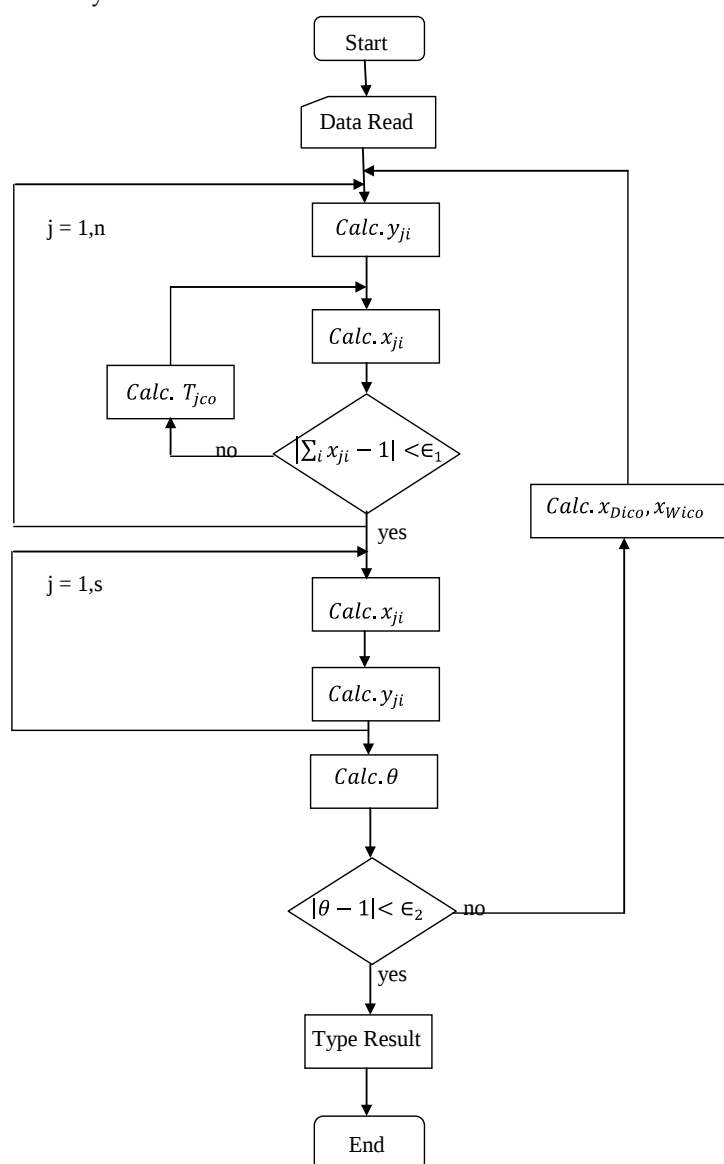


FIGURE 2 FLOW CHART FOR SOLVING THE OPERATION TYPE OF MULTICOMPONENT DISTILLATION PROBLEM.

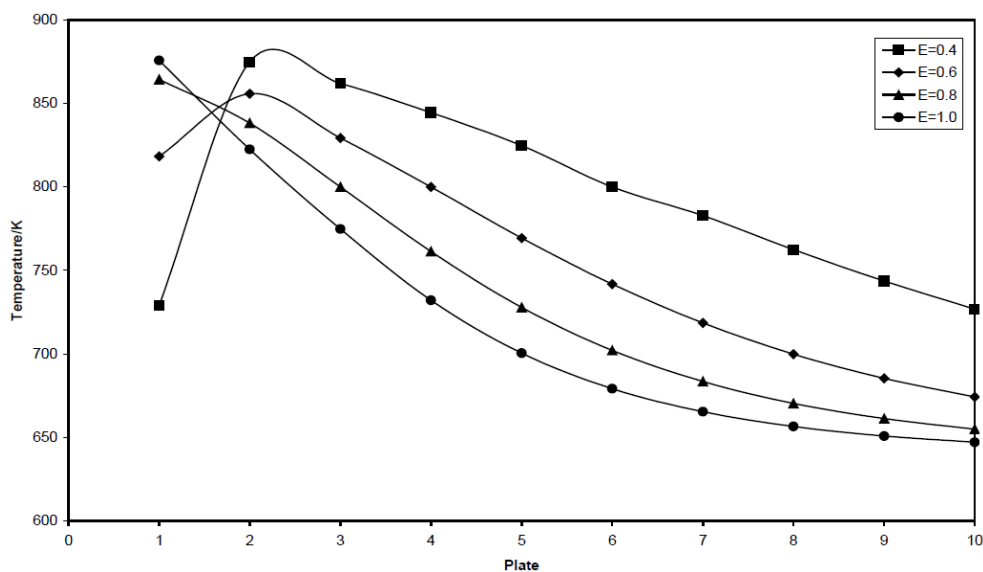


FIGURE 3 TEMPERATURE PROFILE IN THE DISTILLATION COLUMN AT DIFFERENT MURPHREE PLATE EFFICIENCIES

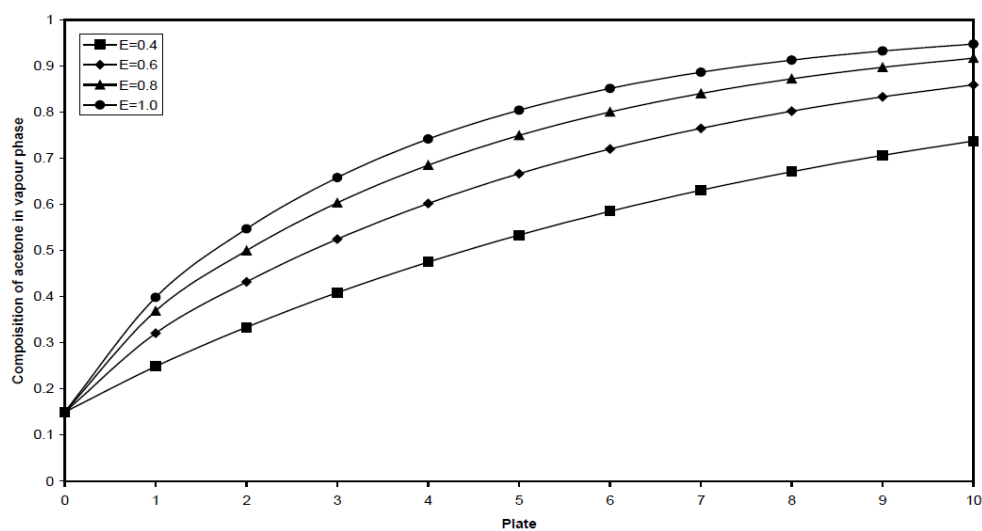


FIGURE 4 LIQUID-PHASE COMPOSITION OF ACETONE IN ACETONE-CHLOROFORM-METHANOL SYSTEM DOWN THE COLUMN AT DIFFERENT MURPHREE PLATE EFFICIENCIES

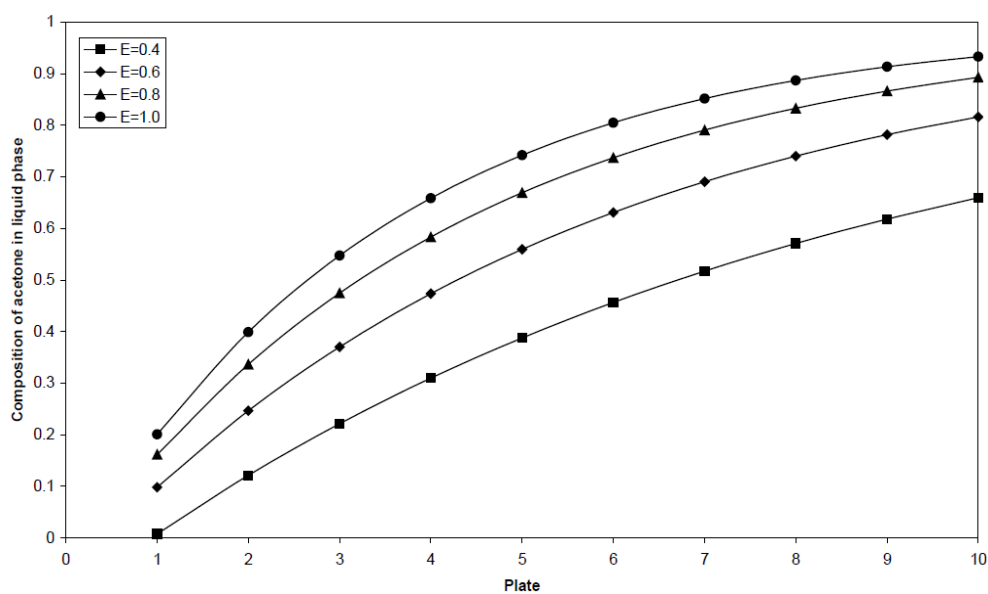


FIGURE 5 LIQUID-PHASE COMPOSITION OF CHLOROFORM IN ACETONE-CHLOROFORM-METHANOL SYSTEM DOWN THE COLUMN AT DIFFERENT MURPHREE PLATE EFFICIENCIES

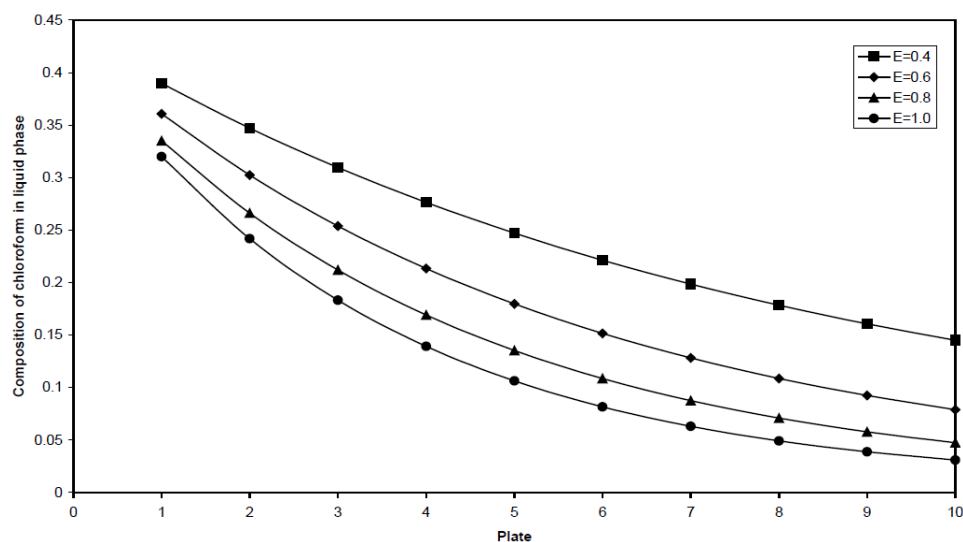


FIGURE 6 LIQUID-PHASE COMPOSITION OF METHANOL IN ACETONE-CHLOROFORM-METHANOL SYSTEM DOWN THE COLUMN AT DIFFERENT MURPHREE PLATE EFFICIENCIES

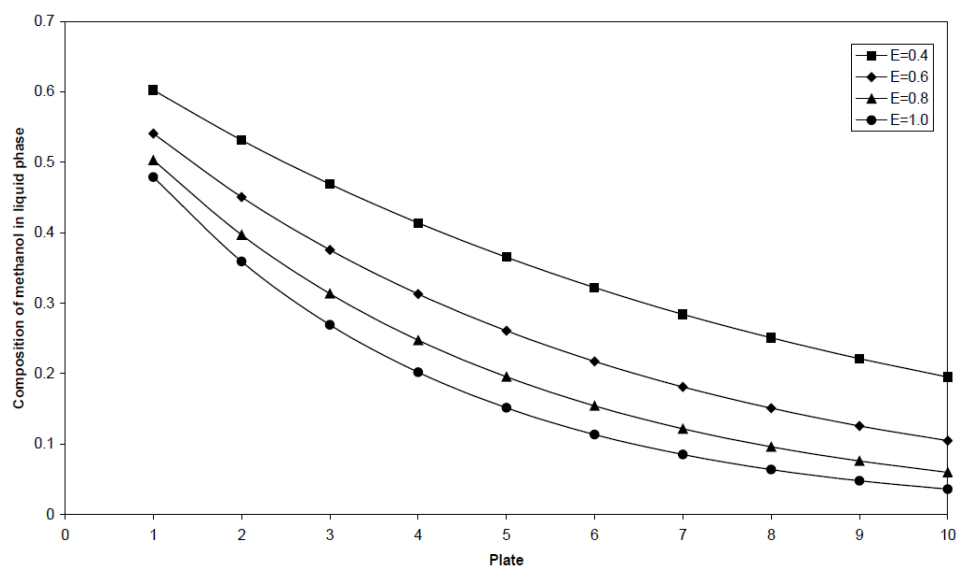


FIGURE 7 VAPOUR-PHASE COMPOSITION OF ACETONE IN ACETONE-CHLOROFORM-METHANOL SYSTEM DOWN THE COLUMN AT DIFFERENT MURPHREE PLATE EFFICIENCIES

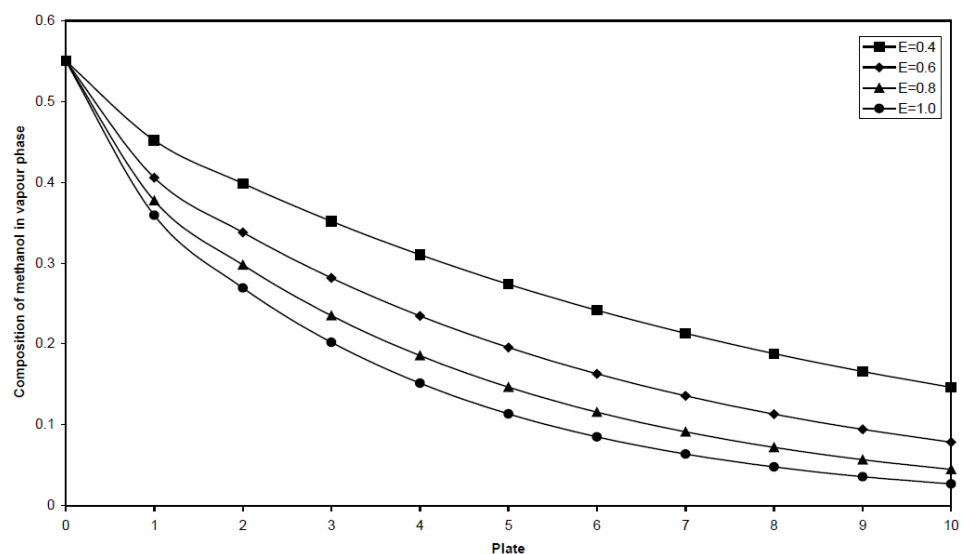


FIGURE 8 VAPOUR-PHASE COMPOSITION OF CHLOROFORM IN ACETONE-CHLOROFORM-METHANOL SYSTEM DOWN THE COLUMN AT DIFFERENT MURPHREE PLATE EFFICIENCIES

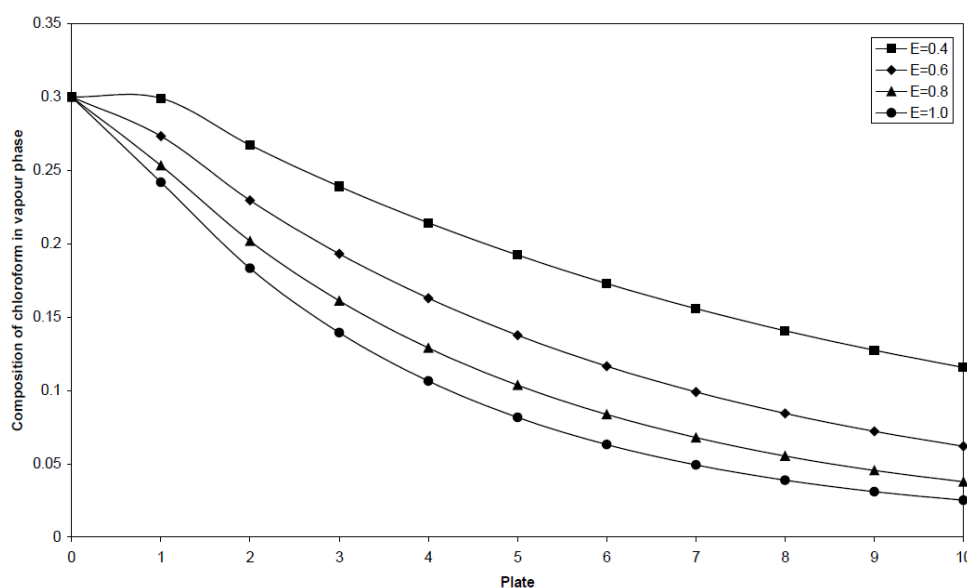


FIGURE 9 VAPOUR-PHASE COMPOSITION OF METHANOLL IN ACETONE-CHLOROFORM-METHANOL SYSTEM DOWN THE COLUMN AT DIFFERENT MURPHREE PLATE EFFICIENCIES

Simulation Result and Discussion

The model equations developed for the operation type of a distillation column were applied to a ternary system of acetone-chloroform-methanol, which were referred to as components 1, 2 and 3 respectively. The model equations were solved using an in-built program in MATLAB. An algorithm for solving the operation type of multicomponent distillation problem is shown in Figure 2. The input data are shown in Table 1.

TABLE 1 INPUT SPECIFICATIONS FOR ACETONE-CHLOROFORM-METHANOL SYSTEM.

Component	$z_{j,F}$	Antoine's constants		
		A_i	B_i	C_i
Acetone (1)	0.2	7.11714	1210.595	229.664
Chloroform (2)	0.3	6.95465	1170.966	226.232
Methanol (3)	0.5	8.08097	1582.271	239.726

The constants for calculation of non-ideality are (Perry et al., 1999; Prausnitz, 1999):

$$A_{1,2}=0.69, A_{1,3}=0.519, A_{2,1}=0.83,$$

$$A_{2,3}=1.80, A_{3,1}=0.701, A_{3,2}=0.715$$

and $Q' = -0.368$.

In the application of the proposed method, a feed of 100 mol/h containing 20 mol % methanol, 30 mol % chloroform and 50 mol % methanol is to be fractionated in a distillation column operating at atmospheric pressure of 760 mmHg, with fractional recovery of acetone and chloroform in the distillate

being 0.99 and 0.01 respectively. The distillate is 20 mol/h. The total number of theoretical stages in the column is 10. The parameters used in obtaining simulated results are as follows: $F=100$ mol/h, $D=20$ mol/h, $x_{D,1}=0.99$, $x_{D,2}=0.01$, $N=10$, $0.4 \leq E_{j,k}^{MV} \leq 1.0$, reflux ratios at the top and bottom of the column are $R=3.0$ and $R^*=2.5$ respectively, and boundary condition at the condenser, $Y_1 = [0.15 \ 0.30 \ 0.55]$.

Figure 3 shows the temperature variation in the distillation column as one cascade down the column. From stages 1 to 2, temperature increases for $E_{j,k}^{MV}=0.4$ and 0.6 and then decreases onwards to stage 10 while for $E_{j,k}^{MV}=0.8$ and 1.0, a decrease in temperature down the column from stages 1 to 10 was observed.

Figures 4 and 7 show the respective increasing liquid-phase and vapour-phase compositions of acetone (in the ternary system of acetone-chloroform-methanol) down the column at different Murphree plate efficiencies between 0.4 and 1.0. This is indicative of the fact that acetone is the most volatile component.

The liquid-phase and vapour-phase compositions of chloroform and methanol in the ternary system decreased down the column at different Murphree efficiencies between 0.4 and 1.0 as shown in Figures 5 and 8; and 6 and 9 respectively. Methanol is the least volatile component with chloroform as the intermediate.

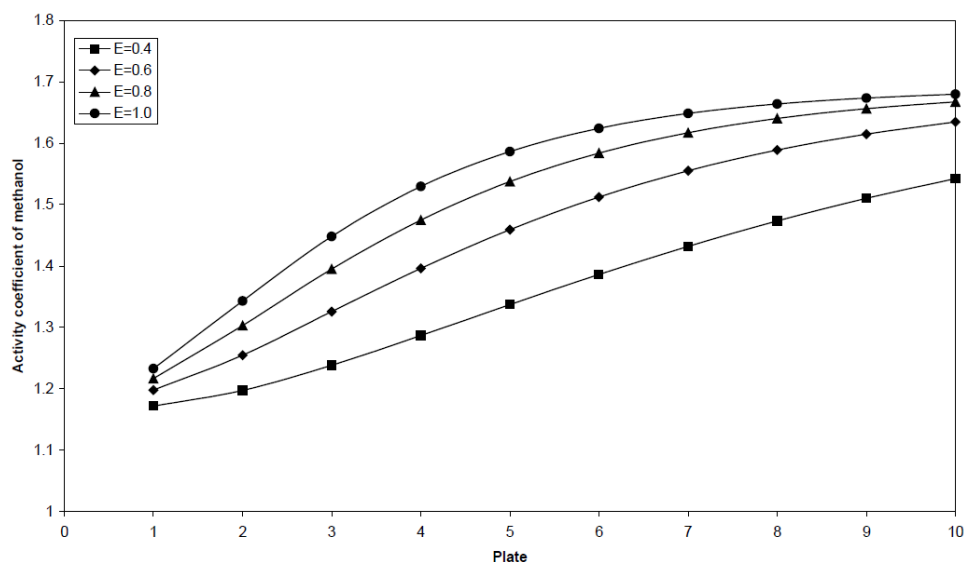


FIGURE 10. VARIATION OF ACTIVITY COEFFICIENT OF ACETONE IN ACETONE-CHLOROFORM-METHANOL SYSTEM WITH STAGES

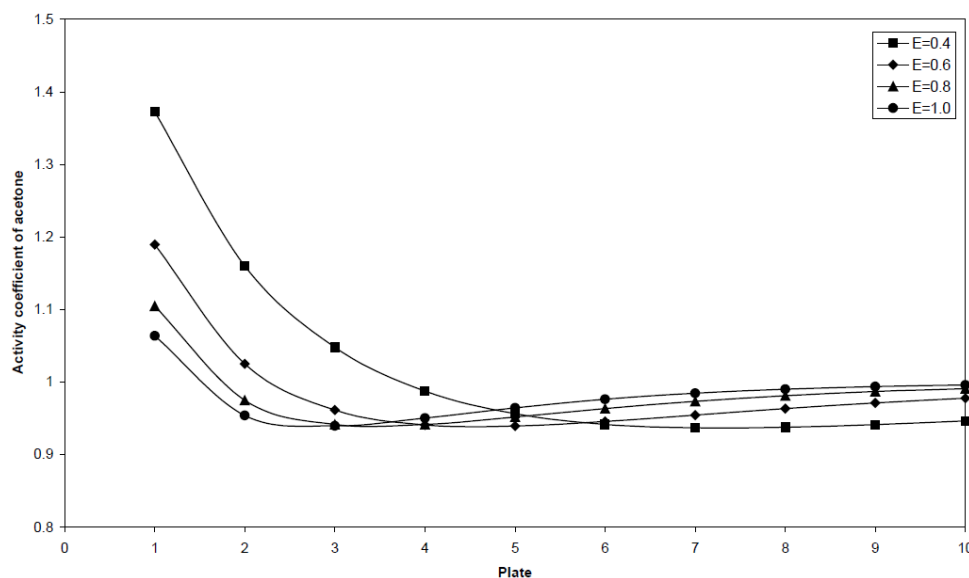


FIGURE 11 VARIATION OF ACTIVITY COEFFICIENT OF CHLOROFORM IN ACETONE-CHLOROFORM-METHANOL SYSTEM WITH STAGES

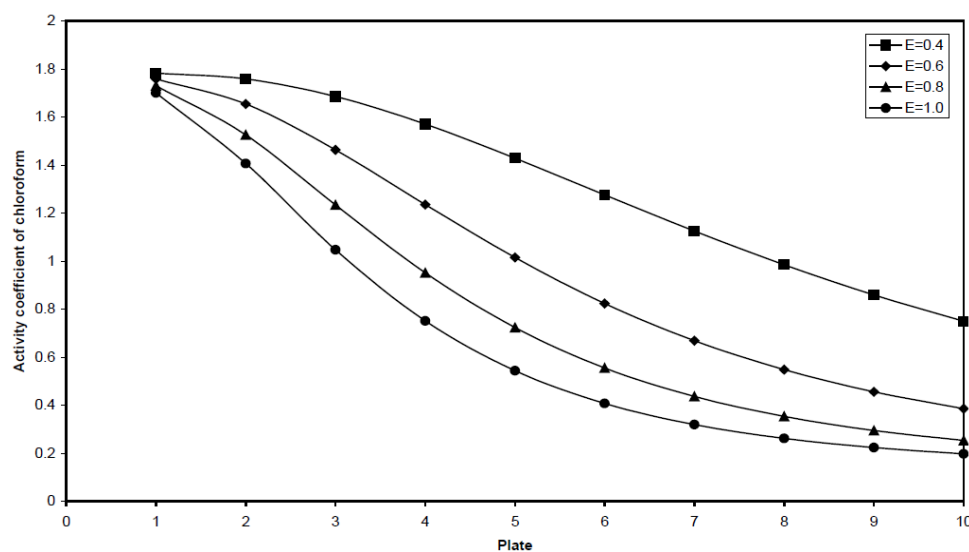


FIGURE 12 VARIATION OF ACTIVITY COEFFICIENT OF METHANOL IN ACETONE-CHLOROFORM-METHANOL SYSTEM WITH STAGES

Figures 10-12 show the variation of activity coefficient of the components with number of theoretical stages in the distillation column. It is seen that the activity coefficients of acetone and chloroform decrease down the column, with the former levelling off for $0.4 \leq E_{j,k}^{MV} \leq 1.0$ while the activity coefficient of methanol increases down the stage. The activity coefficient (non-ideality) explains the escaping tendency of a component relative to Raoult's law in vapour-liquid equilibrium. Methanol thus shows a positive deviation from Raoult's law throughout the column.

In the simulated results presented, convergence was achieved within 7–10 iterations, which is indicative of the fact that the method of convergence used in this study is best appropriate for the ternary system of acetone, chloroform and methanol.

Conclusions

Multicomponent distillation column has been modelled using plate-to-plate method involving the Murphree plate efficiency and simulated using MATLAB program. The calculations were initiated with the boundary condition at the condenser. However, further work is required to nullify the assumption of constant molar overflow. This removes the incorporation of the enthalpy balance equation. The method is simple with fast convergence achievement but there is a need for integrating a search method with the main program for finding an optimum feed stage based on some appropriate objective function.

Notation

$A_{j,n}$	Margule's constant (constant of non-ideality), dimensionless
D	molar rate of distillate, mol/h
$E_{j,n}^{MV}$	Murphree plate efficiency, dimensionless
F	molar rate of feed, mol/h
K	distribution coefficient, dimensionless
M	total number of components, dimensionless
N	total number of theoretical plates in the column, dimensionless
n	number of plates in enriching section, dimensionless
W	molar rate of bottoms, mol/h
x_i	mol fraction of component i in bottoms,

dimensionless

y_i mol fraction of component i in distillate, dimensionless

z_i mol fraction of component i in feed, dimensionless

Greek Symbols

γ_i	activity coefficient of component i
θ	correction factor for convergence

Subscripts

as	assumed value
cal	calculated value
co	corrected value
f	feed plate
j	component

Superscripts

*	stripping section
s	number of plates in stripping section
o	saturation condition

REFERENCES

- Brooks, B. A. (1993). *Modelling of a Distillation Column Using Bond Graphs*, M. Sc. Thesis, University of Arizona, 70-88.
- Fidkowski, Z. T., Malone, M. F. and Doherty, M. F. (1991). Non-Ideal Multicomponent Distillation: Use of Bifurcation Theory for Design, *AIChE Journal*, 37, 1761-1768.
- Frau, A., Baratti, R. and Alvarez, J. (2010). *Estimation Model Design for a Multicomponent Distillation Column with Temperature Measurements*, 20th European Symposium on Computer Aided Process Engineering, Istanbul, Turkey.
- Hass, J. R. (1992). *Rigorous Distillation Calculations in Distillation Design*, McGraw-Hill, New York.
- Holland, C. D. and Liapis, A. I. (1983). *Computer Methods for Solving Dynamic Separation Problems*, McGraw-Hill, New York.
- Jimenez, L., Basualdo, M., Gomez, J.C. and Rosa, M. (2002). Non-Linear Dynamic Modelling of Multicomponent Batch Distillation, *Brazilian Journal of Chemical Engineering*, 19(3), 307-317.
- Julka, V. and Doherty, M. F. (1993). Geometric Non-Linear

- Analysis of Multicomponent Non-Ideal Distillation: A Simple Computer Aided Design Procedure, *Chem. Eng. Sci.*, 48, 1367-1375.
- Ketchum, R. G. (1979). A Combined Relaxation-Newton Method: A New Global Approach to the Computation of Thermal Separation Processes, *Chem. Eng. Sci.*, 34, 387-397.
- Levy, S. G., Van Dongen, D. B. and Doherty, M. F. (1985). Design and Synthesis of Homogeneous Azeotropic Distillation and Minimum Reflux Calculations for Non-Ideal Azeotropic Columns, *Ind. Eng. Chem. Fundam.*, 24, 463.
- Lewis, W. K. and Matheson, G. L. (1932). Studies in Distillation Design of Rectifying Columns for Natural and Refinery Gasoline, *Ind. Eng. Chem.*, 24, 494.
- Minh, V. T. and Abdul Rani, A. M. (2009). Modelling and Control of Distillation Column in a Petroleum Process, *Mathematical Problems in Engineering*, 2(14), 40-47.
- Perry, R. H, Green, D. W. and Maloney, J. O. (1999). *Chemical Engineers' Handbook*, Seventh Edition, McGraw-Hill Book Co., New York.
- Popoola, L. T., Babagana, G. and Susu, A. A. (2013). A Review of an Expert System Design for Crude Oil Distillation Column Using the Neural Networks Model and Process Optimization and Control Using Genetic Algorithm Framework, *Advances in Chemical Engineering and Science*, 3, 164-170.
- Prausnitz, J. M. (1999). *Molecular Thermodynamics of Fluid-Phase Equilibria*, Third Edition, 237-793.
- Rao, D. P., Ashok, K., Davendra, A. and Abhishek, S. (2005). A Simple Design Method for Multicomponent Distillation Columns, *Chem. Eng. Sci.*, 48, 1367-1371.
- Rose, A., Sweeny, R. and Schrodt, V. (1958). Continuous Distillation Calculations by Relaxation Method, *Ind. Eng. Chem.*, 50, 737.
- Solomon, A. F. (1981). *Recent Advances in the Study of Multicomponent Distillation*, B. Sc. Thesis, Chemical Engineering Department, University of Lagos, Nigeria.
- Thiele, E. W. and Geddes, R. L. (1933). Computation of Distillation Apparatus for Hydrocarbon Mixtures, *Ind. Eng. Chem.*, 25, 289-295.
- Thong, D. Y. and Jobson, A. S. (2001). Multicomponent Homogeneous Azeotropic Distillation and Column Design, *Chem. Eng. Sci.*, 56, 4393-4399.
- Thong, D. Y., Castello, F. J. and Towler, G. P. (2000). Distillation Design and Retrofit using Stage-Composition Lines, *Chem. Eng. Sci.*, 5, 625-637.
- Truong, H. S., Ismail, I. and Razali, R. (2011). *Fundamental Modelling and Simulation of a Binary Continuous Distillation Column*, Electrical and Electronic Eng. Dept., Universiti Teknologi, Malaysia.
- Wohl, K. (1946). Application of Margules' Equation to Ternary Systems, *Trans. Ame. Inst. Chem. Engrs.*, 42, 215-223.
- Yamada, I., Suda, S. and Hiraoka, S. (1980). An Algorithm for Solving the Operation Type of Multicomponent Distillation Problem, *Journal of Chem. Eng. of Japan*, 13, 6-15.
- Zuzana, S., Labovsky, J., Markos, J. and Jetemensky, L. (2007). *Impact of Mathematical Model Selection on Production of Steady State Behaviour of a Reactive distillation Column*, 17th European Symposium on Computer Aided Process Engineering, Istanbul, Turkey.